FOLDER: CDMCMC

File Name

ControlData.m
FemaleData.m
MaleData.m
Kidney2009.m
humandata.m
MMouse_liver_mcmcKG.m
HumanLiverMCMCrun.m
HumanLungMCMCrun.m
FMouseLiverMCMC1lvl.m
MMouseLiverMCMC1lvl.m
FMouse_lung_mcmcrun.m
MMouse_lung_mcmcrun.m
FMouse_KidneyMCMC1lvlvk.m
FMouseKidneyMCMC1lvl.m
MMouseKidneyMCMC1lvl.m
FRatLiverMCMCrun.m
MRatLiverMCMCrun.m
FRatLungMCMCrun.m
MRatLungMCMCrun.m
FRatKidneyMCMC1lvl.m
MRatKidneyMCMC1lvl.m
female_mouse_liver.m
female_mouse_lung.m
female_mouse_kidney.m
male_mouse_liver.m
male_mouse_lung.m
male_mouse_kidney.m
Female_rat_liver.m
Female_rat_lung.m
Female_rat_kidney.m
Male_rat_liver.m
Male_rat_lung.m
Male_rat_kidney.m
mixed_human_liver.m
mixed_human_lung.m

Notes:

FOLDER: CDMCMC\MCMCScripts

fminvitroliv1lvl.m
invitroflivmcrd.m
invitromc12frl.m
invitromc12mrl.m
invitromc13hl.m

invitromcmc11h.m
invitromlivmcrd.m
mminvitroliv1lvl.m

Notes

FOLDER: MCMCout

Female_Mouse_MCMC.R
Male_Mouse_MCMC.R
Female_rat_MCMC.R
Male_rat_MCMC.R
Human_MCMC.R

Notes:

Description

Control Data used for RLOSS in the MCMC model (adds variability to background loss)
Female Data used in MCMC analysis and plotting of posterior for female mouse and rat
Male Data used in MCMC analysis and plotting of posterior for male mouse and rat
Kidney Data used in MCMC and plotting for mouse and rat (both sexes)
Human Data used for MCMC and human plotting
Male mouse liver MCMC - used to estimate vmax and kg with km fixed to 1.0 mg/L (establishes kg)
Human liver MCMC - used to estimate vmax and km for the mixed human microsomal incubation
Human lung MCMC - used to estimate vk for the mixed human lung microsomal incubation
female mouse liver - used to estimate vmax and km for female mouse liver microsomal incubation
Male mouse liver - used to estimate vmax and km for male mouse liver microsomal incubation
female mouse lung - used to estimate vmax and km for female mouse lung microsomal incubation
Male mouse lung - used to estimate vmax and km for male mouse lung microsomal incubation
female mouse kidney - used to estimate vk for female mouse kidney microsomal incubation
female mouse kidney - file not used to estimate vmax and km for female mouse kidney microsomal incubation (fai
Male mouse kidney - used to estimate vmax and km for male mouse kidney microsomal incubation
female rat liver - used to estimate vmax and km for female rat liver microsomal incubation
Male rat liver - used to estimate vmax and km for male rat liver microsomal incubation
female rat lung - used to estimate vmax and km for female rat lung microsomal incubation
Male rat lung - used to estimate vmax and km for male rat lung microsomal incubation
female rat kidney - file used to estimate vmax and km for female rat kidney microsomal incubation
Male rat kidney - used to estimate vmax and km for male rat kidney microsomal incubation
Simulates and plots posterior geometric mean from mcmc for female mouse liver
Simulates and plots posterior geometric mean from mcmc for female mouse lung
Simulates and plots posterior geometric mean from mcmc for female mouse kidney
Simulates and plots posterior geometric mean from mcmc for male mouse liver
Simulates and plots posterior geometric mean from mcmc for male mouse lung
Simulates and plots posterior geometric mean from mcmc for male mouse kidney
Simulates and plots posterior geometric mean from mcmc for female rat liver
Simulates and plots posterior geometric mean from mcmc for female rat lung
Simulates and plots posterior geometric mean from mcmc for female rat kidney
Simulates and plots posterior geometric mean from mcmc for male rat liver
Simulates and plots posterior geometric mean from mcmc for male rat lung
Simulates and plots posterior geometric mean from mcmc for male rat kidney
Simulates and plots posterior geometric mean from mcmc for mixed human liver
Simulates and plots posterior geometric mean from mcmc for mixed human lung

1) The order of the MCMC file runs was Mmouse_liver_mcmcKG.m first to establish Kg which was fixed in other m
2) M-files that establish the prior distributions and likelihoods are in a sub-folder of this model (MCMCscripts). The
3) Simulation m-files listed here can be run in any order at this time as the Kg is set to 0.45 L/hr from the analysis a

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Female Mouse and Rat Liver and Kidney
Female Mouse Liver
Female Mouse Kidney, Female Rat Lung
Male Rat Lung
Human Lung

Human Liver
Male Mouse Liver
Male Mouse Kidney, Liver, Lung, Male Rat Kidney and Liver

1) Each file is associated with two additional files (.mc and .mcx) located in the MCMCScripts folder

Contains script to load and analyze the three chains for female mouse in vitro posteriors
Contains script to load and analyze the three chains for male mouse in vitro posteriors
Contains script to load and analyze the three chains for female rat in vitro posteriors
Contains script to load and analyze the three chains for male rat in vitro posteriors
Contains script to load and analyze the three chains for mixed human in vitro posteriors

1) Each file contains script for all tissues analyzed; male mouse includes the additional liver analysis that establishe
2) Three data files (.dat) from the separate chains are included for each species/sex/tissue combination
3) Requires R packages "coda" and "readr"

nd the posterior geometric means are set in the plot files.